

AD-A065 110

WISCONSIN UNIV-MILWAUKEE DEPT OF CHEMISTRY

INTERNATIONAL SUMMER INSTITUTE IN SURFACE SCIENCE (3RD) (ISISS --ETC(U)

FEB 79 R VANSELOW

F/6 7/4

N0014-77-G-0058

NL

UNCLASSIFIED

1 OF 1  
AD  
A065110



END  
DATE  
FILMED  
4 -79  
DDC

AD A0 65110

DDC FILE COPY

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

**LEVEL II**

**12**

| REPORT DOCUMENTATION PAGE  |  | READ INSTRUCTIONS<br>BEFORE COMPLETING FORM       |
|--|--|---|
| 1. REPORT NUMBER<br>N0014-77-G-0058  | 2. GOVT ACCESSION NO.<br>(3rd)   | 3. RECIPIENT'S CATALOG NUMBER<br>5                |
| 4. TITLE (and Subtitle)<br>Third International Summer Institute in<br>Surface Science (ISSISS 1977).   | 5. TYPE OF REPORT & PERIOD COVERED<br>9 Final rept.<br>1 Aug 77-30 Apr 78    | 6. PERFORMING ORG. REPORT NUMBER                  |
| 7. AUTHOR(s)<br>Professor Ralf/Vanselow  | 8. CONTRACT OR GRANT NUMBER(s)<br>15 ✓ N0014-77-G-0058                       |   |
| 9. PERFORMING ORGANIZATION NAME AND ADDRESS<br>University of Wisconsin-Milwaukee<br>Milwaukee, Wisconsin 53201   | 10. PROGRAM ELEMENT, PROJECT, TASK<br>AREA & WORK UNIT NUMBERS<br>NR 392-025 |   |
| 11. CONTROLLING OFFICE NAME AND ADDRESS<br>Office of Naval Research<br>Arlington, Va. 22217  | 12. REPORT DATE<br>11/20 February 1979                                       | 13. NUMBER OF PAGES<br>14                         |
| 14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)<br>ONR Branch Office - Chicago<br>536 So. Clark Street<br>Chicago, Illinois 60605  | 15. SECURITY CLASS. (of this report)<br>Unclassified<br>12 16p.              | 15a. DECLASSIFICATION/DOWNGRADING<br>SCHEDULE N/A |
| 16. DISTRIBUTION STATEMENT (of this Report)<br>Distribution of this document is unlimited.   |  |   |
| 17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)<br>Distribution of the abstract is unlimited.   |  |   |
| 18. SUPPLEMENTARY NOTES<br>Published in: CRC-Critical Reviews in Solid State<br>and Materials Sciences 7 (2) (3) (4), 81-384 (1978)<br>8 (1) (2), 1-244 (1978)   |  |   |
| 19. KEY WORDS (Continue on reverse side if necessary and identify by block number)<br>ISSISS 1977, Chemisorption, Physisorption, Statistical Thermo-<br>dynamics of Adsorption, Theory of Desorption, Surface Segregation,<br>Computer Simulation of Adsorption, Surface Migration, Epitaxy,<br>Techniques for Surface Analysis, Catalysis, Industrial Surface<br>Science.   |  |   |
| 20. ABSTRACT (Continue on reverse side if necessary and identify by block number)<br>At the third International Summer Institute in Surface Science,<br>twenty-one leading scientists presented tutorial review talks on<br>gas-solid interfaces. Paper topics: "Historical Review: Chemisorp-<br>tion on Metals-Retrospect and Prospect," "Surface Reactions at<br>High Pressures," "Chemisorption-Island Formation and Adatom Inter-<br>actions," "Theory of Interaction Between Chemisorbed Atoms," "Prop-<br>erties of Single Atoms on Metal Surfaces," "Photoelectron |  |   |

DDC

MAR 1 1979

D

DD FORM 1473 1 JAN 73

EDITION OF 1 NOV 65 IS OBSOLETE  
S/N 0102-014-6601

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

79 02 26 074 409760

Jim

20. (continued)

Spectroscopy of Adsorption Layers," Structure, Bonding and Reactivity of Polymer Surfaces Studied by Means of ESCA," Atomic Geometry of Semiconductor Surfaces," "Compositional Depth Profiling by Auger Electron Spectroscopy," "Modification of the Strength of Solids by Chemisorption," "Chemical Reactions on Single Crystal Metal Surfaces," "Analogies Among Chemical Properties of Metal Surfaces, Organometallic Molecules and Enzymes," "Photodesorption," "Recent Applications of Field Emission Microscopy," "Neutron Diffraction by Adsorbed Monolayers," "Long Range Order in Two Dimensions," "Computer Simulation of Adsorption," "The Theory of Desorption," "Kinetics of Adsorption, Desorption and Migration on Single Crystal Metal Surfaces," "The Role of Lattice Misfit in Epitaxy," "Segregation to Surfaces: Dilute Alloys of the Transition Metals."

|                                 |   |
|---------------------------------|---|
| ACCESSION for                   |   |
| DTIC                            | Write Section <input checked="" type="checkbox"/> |
| DDI                             | Diff Section <input type="checkbox"/>             |
| UNANNOUNCED                     | <input type="checkbox"/>                          |
| JUSTIFICATION.....              |   |
| BY.....                         |   |
| DISTRIBUTION/AVAILABILITY CODES |   |
| Dist.                           | AVAIL. and/or SPECIAL                             |
| A                               |   |

79 02 26

074



Report N0014-77-G-0058

THIRD INTERNATIONAL SUMMER INSTITUTE IN SURFACE SCIENCE  
(ISISS 1977)

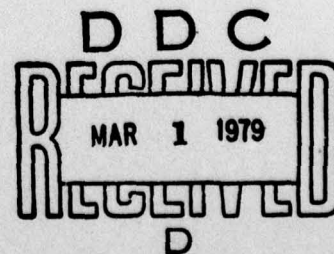
Professor Ralf Vanselow, Director  
Department of Chemistry  
University of Wisconsin-Milwaukee  
Milwaukee, Wisconsin 53201

Final Report for the period August 1, 1977 - April 30, 1978

Prepared for

OFFICE OF NAVAL RESEARCH  
Arlington, Va. 22217

ONR BRANCH OFFICE - CHICAGO  
536 So. Clark Street  
Chicago, Ill. 60605





The academic goals of ISISS were outlined in the editorial comments of "Surface Science: Recent Progress and Perspectives (ISISS 1975):"

"The favorable acceptance of ISISS was gratifying, but did not exactly come as a surprise. During the recent decade, advanced ultrahigh vacuum technology has made the achievement of pressures  $< 10^{-10}$  Torr a routine operation so that surfaces, once freed from impurities, can be kept clean over a sufficient length of time and adsorbates then can be admitted at well-dosed amounts. Techniques for surface analysis were more and more refined; with the atom probe we are now able to analyze even single surface atoms or chemical complexes. Progress in the theory of the solid state subsequently allowed some fruitful dealing with the theoretical aspects of solid surfaces. All these developments combined with the demand for data by vital branches of our modern technology, caused an increasing flood of publications especially in the field of gas-solid interfaces. It became hard to catch up with the literature in one's own narrow area and it appeared nearly impossible to keep track of the developments in neighboring fields. As in other fast developing parts of the natural sciences, one consequently observes some isolationism and the appearance of communication problems. It is quite clear that such a tendency, where one no longer learns from progress or setbacks in neighboring areas, would be very much to our disadvantage. To counteract this tendency, ISISS was organized. Leading experts from various subdivisions of surface science - we chose to restrict the topics to gas-solid interfaces - presented tutorial review talks in which recent progress was summarized and future trends were pointed out."

In order to keep ISISS 1977 at a level of highest quality all former ISISS speakers were invited to suggest names of suitable lecturers. To avoid duplication, none of the lecturers of the 1975 Summer Institute were invited to present a paper. The final list showed twenty-one internationally known experts in the field of gas-solid interfaces. The speakers came from Germany, Israel, the Republic of South Africa, the United Kingdom, and from the U.S.A.

The following list shows their names, their affiliations, topics, and short summaries of the papers presented.

J. L. Beeby, University of Leicester, U.K.

The Theory of Desorption

A critical review is presented of the theory of desorption from surfaces. A simple one-dimensional classical model is presented by way of illustration and carefully analysed. Deviations from the simple result, including dissipative effects and non-harmonic potentials, are introduced. The changes required for quantum mechanical calculations are outlined. Finally, some brief remarks are made on the theory of flash desorption.

J. M. Blakely, Cornell University

Segregation to Surfaces: Dilute Alloys of the Transition Metals

The theoretical basis for component segregation to interfaces in alloys is briefly reviewed. Macroscopic thermodynamic analyses are covered as well as treatments based on model isotherms. Experimental work on the segregation of carbon to free surfaces of Ni and Pt single crystals is discussed. This work demonstrates the dependence of segregation behavior on surface structure. Examples are given of (1) quasi-Langmuir behavior, (2) surface phase condensation, (3) the absence of segregation, and (4) segregation-induced reconstruction. The types of experiments which need to be done are also discussed.

David T. Clark, University of Durham, U.K.

Structure, Bonding and Reactivity of Polymer Surfaces Studied by Means of ESCA

The large range of available information levels from the ESCA experiment endows the technique with wide-ranging capability in the investigation of many aspects of the surface science of polymeric materials. After a brief consideration of background information of particular relevance to application in the polymer field, detailed consideration is given to representative examples which illustrate the important role which ESCA can play in elaborating details of the structure, bonding, and reactivity of polymer surfaces.



Charles B. Duke, Xerox Corporation, N.Y.

### Atomic Geometry of Semiconductor Surfaces

The article provides a review of structure determinations of semiconductor surfaces via analyses of elastic low-energy electron diffraction (ELEED) intensities. Inspection of the observed spot patterns reveals that all low-index surfaces of silicon and germanium, together with the polar surfaces of zincblende and wurtzite compound semiconductors, exhibit reconstructions which alter the space group symmetry of the surface relative to that expected for an ideally terminated bulk crystal. The electrically neutral (nonpolar) cleavage faces of zincblende, wurtzite, rocksalt, and molybdenite compound semiconductors exhibit spot patterns consistent with the bulk space group symmetry. Analysis of the ELEED intensities reveals, however, that they also may be reconstructed. In the case of certain faces of the tetrahedrally coordinated semiconductors (i.e., zincblende  $\{110\}$  and wurtzite  $\{10\bar{1}0\}$ ), the cation is shifted inward and the anion either outward or inward. Moreover, the reconstructions seem to penetrate to at least the third and fourth atomic layers in all of the tetrahedrally coordinated semiconductors, including group IV elements. Small layer spacing contractions occur for  $\text{MoS}_2\{0001\}$ ,  $\text{NbSe}_2\{0001\}$ ,  $\text{ZnO}\{11\bar{2}0\}$ ,  $\text{MgO}\{100\}$ , and  $\text{NiO}\{100\}$  are thought to exhibit almost the truncated bulk geometry. These structures are consistent with the concept that the reconstructions are largest for materials exhibiting covalent bonding at surfaces for which the symmetry restrictions on the surface atom motions are least severe. A synopsis and critique of the ELEED intensity analysis surface structure determination methodology as applied to semiconductor surfaces are presented. Results obtained by this methodology are compared with those emanating from comparisons of calculated surface state eigenvalue spectra and densities of valence states (DOVS) with measured photoemission, electron energy loss, and ion-neutralization spectra. Intrinsic uncertainties in the ELEED methodology are shown to be  $\Delta d \sim 0.1\text{\AA}$  whereas those in the DOVS-surface-state methodology are estimated to be  $\Delta d \sim 0.4\text{\AA}$ . The two methodologies yield compatible results for  $\text{GaAs}\{11\bar{0}\}$  and  $\text{Si}(111)\text{-p}(1\times 1)$ , but not for  $\text{Si}(100)\text{-p}(2\times 1)$ . The latter discrepancy probably is not significant because too limited a structural search was performed in both sets of calculations. Presently available structural parameters are tabulated for all systems that have been examined to date (i.e.,  $\text{LiF}\{100\}$ ,  $\text{MgO}\{100\}$ ,  $\text{NiO}\{100\}$ ,  $\text{ZnO}\{0001\}$ ,  $\text{ZnO}\{10\bar{1}0\}$ ,  $\text{ZnO}\{11\bar{2}0\}$ ,  $\text{GaAs}\{110\}$ ,  $\text{ZnSe}\{110\}$ ,  $\text{Si}(100)\text{-p}(2\times 1)$ ,  $\text{Si}(111)\text{-p}(1\times 1)$ ,  $\text{Si}(111)\text{-p}(2\times 1)$ ,  $\text{Si}(111)\text{-p}(7\times 7)$ ,  $\text{MoS}_2\{0001\}$ , and  $\text{NbSe}_2\{0001\}$ ).

Theodore L. Einstein, University of Maryland

### Theory of Interaction Between Chemisorbed Atoms

A general review of the theory of the various forms of interactions, both electron and lattice induced, between chemisorbed atoms is presented. Particular care is given to the calculations of the indirect electronic



interaction between two adatoms on substrates modeling the properties of transition metals. The roles of self-consistency and correlation are seen to be less important than in single-atom adsorption, but the level of accuracy attainable is also lower than in the one-adatom or monolayer problems. Within the framework of a single simple model, two-adatom, three-adatom, and ordered-overlayer effects are compared. The associated changes in density of states are briefly considered. Applications are made to the lattice gas model of adatoms. In particular, the two kinds of disordering transitions and the shape of adatom islands at low coverages are discussed. The appendix contains a review of calculations of the indirect interaction in the asymptotic regime, which generally lies beyond the interadatom separations at which the interaction is physically important. Conclusions and ideas about directions in which the field should be developed are presented.

Robert Gomer, The University of Chicago

#### Recent Applications of Field Emission Microscopy

A brief discussion of the principles of field emission and of field emission microscopy is presented. This is followed by a general discussion of applications, which includes the determination of work function changes in adsorption, the study of the kinetics of adsorption and desorption, the study of surface diffusion, the use of field emitters as gas detectors, and a very brief summary of the electron optical properties of emitters. Next, a more detailed discussion of field emission spectroscopy is given, that is, the measurement of the energy distribution of field-emitted electrons in the absence and presence of adsorbates, which reveals information on the electronic structure of adsorption complexes. Finally, a more detailed discussion of the use of field emission microscopy for the study of adsorbate diffusion is given, including visual measurements which give averages over the emitter and a new method by which diffusion coefficients on individual planes can be determined from the time correlation function of current fluctuations, which is related to that of density fluctuations.

Yoseph Imry, Tel Aviv University, Israel

#### Long Range Order in Two Dimensions

The long-range ordering of continuous-symmetry 2D systems is discussed with particular reference to the case of a nonregistered adsorbed surface layer. It is demonstrated that while no strict long-range order can exist, there should be a low-temperature phase where the order parameter correlations decay slowly in space and time. This will cause the results of, for example, X-ray and neutron scattering and Mössbauer measurements to differ only subtly from those in truly ordered systems. However, careful measurements of line shapes and the dependence of size may yield the typical 2D correlations. The physical reasons for the validity of the low-temperature approximations are discussed, and the situation at higher temperatures, including the transition point, is reviewed.

Keith H. Johnson, Massachusetts Institute of Technology

Analogies Among Chemical Properties of Metal Surfaces, Organometallic Molecules and Enzymes

Analogies among the chemically active sites of metal surfaces, organometallic molecules, and metalloenzymes are described, using the results of self-consistent-field X-alpha (SCF-X $\alpha$ ) electronic-structure studies of transition-metal coordination complexes and clusters of catalytic and biocatalytic importance. Electronic indices of catalytic activity, based on the concepts of spin-orbital electronegativity and spin-orbital symmetry, are proposed and extracted from the calculated electronic structures. Illustrative examples include: (1) coordinatively unsaturated transition-metal complexes as analogues of active sites on transition-metal surfaces; (2) transition-metal surfaces; (2) transition-metal clusters, with emphases on the relationships among the electronic structure, magnetic properties, and catalytic activity of iron clusters and surfaces; (3) the active centers of iron-sulfur proteins and enzymes as biological analogues of supported metal catalysts.

David A. King, The University of Liverpool, U.K.

Kinetics of Adsorption, Desorption and Migration on Single Crystal Metal Surfaces

In this review, an attempt is made to present an integrated approach towards an understanding of the primary kinetic processes occurring at the gas-metal interface. Techniques for the determination of adsorption, desorption, and migration kinetics are briefly reviewed and evaluated. The steps involved in the formation of a chemisorbed overlayer are examined, with particular attention to the distinction between energy accommodation, trapping into short-lived physisorbed (precursor) states, and adsorption into the chemisorbed state and to the influence of order-disorder phenomena in the chemisorbed overlayer on the rate of formation of that overlayer. Crystallographic anisotropy in adsorption kinetics is discussed in relation to results for nitrogen on tungsten single-crystal planes, and the related phenomena of metastable ("virgin") state formation, conversion to stable states, and activated adsorption are discussed. Available data for surface migration in both the physisorbed and chemisorbed states are briefly reviewed, and the influence of lateral interactions between adatoms on adsorbate mobility is examined in some detail. Finally, the process of thermal desorption is reviewed, with particular attention to the analysis and interpretation of desorption spectra. The marked influence of transitory physisorbed (precursor) states on desorption peak lineshapes, peak temperatures, and apparent desorption order is discussed, and the influence of lateral interactions on the desorption process (producing multiple peak spectra and also affecting the apparent desorption order) is evaluated in relation to recent experimental results.



Max G. Lagally, University of Wisconsin-Madison

Chemisorption-Island Formation and Adatom Interactions

The thermodynamics of island-forming chemisorbed overlayers is reviewed and illustrated with the adsorption of oxygen on the {110} surface of tungsten, with emphasis on experimental aspects. The utility of low-energy electron diffraction (LEED) for studying the surface pair correlation function is described, including a discussion of the instrument response. Measurements of the temperature and coverage dependence of the angular distribution of LEED intensity are related to the size, shape, and order of chemisorbed islands, as well as to phase transitions in these islands. A partial phase diagram of  $W(110)p(2 \times 1)-O$  is presented. Theoretical models to interpret overlayer phase transitions in terms of adatom-adatom interactions are briefly discussed and the results summarized in light of the present status of calculations of such interactions.

Ronald M. Latanision, Massachusetts Institute of Technology

Modification of the Strength of Solids by Chemisorption

Adsorption-induced reductions in the hardness of nonmetallic solids were first reported in 1928 by Rebinder. In the interim, many others have reported that surface active media (long-chain organic compounds, liquid metals, specifically adsorbed ionic species, etc.) affect the plasticity and/or fracture characteristics of a variety of solids including metals, covalent and ionic crystals, silicate glasses, etc. While there have been a variety of explanations for Rebinder effects, such phenomena are not yet well understood. The point of view developed by the Rebinder school is that adsorption-induced softening and strength reduction occur as a consequence of the lowering of the specific free surface energy of the solid, i.e., the work of formation of new surfaces during deformation and fracture. On the other hand, the view pioneered by Westwood and his colleagues is that such phenomena may be understood in a conceptual way from consideration of the type, concentration, mobility, and adsorption-induced redistribution in charge carriers in the solid. While these views are at first glance quite different, they have in common a basis for understanding which is derived from the chemistry and physics of solid-electrolyte interfaces. This discussion will treat the phenomenology and recent explanations of adsorption-induced modifications in the mechanical behavior of solids.

David Lichtman, University of Wisconsin-Milwaukee

Photodesorption

The literature in the field of photodesorption is reviewed. Photodesorption in this paper is related specifically to the quantum process whereby a single bombarding photon leads to the desorption of



an atom or molecule. Material is covered from the early 1950s when the first reports appear through the summer of 1977. Studies have been done on both metal and semiconductor substrates. The reactions on these two kinds of substrates are seen to be quite different. The discussion is, therefore, separated into two major portions. Data on attempts to observe photodesorption from several metal substrates are considered first. The results are summarized and it is concluded that the process is very inefficient on these materials. The second and major part of this paper concerns experimental and theoretical analysis of the photodesorption process from semiconductor substrates. Papers that consider the photodesorption process as such as well as many papers that are of peripheral interest are reviewed. It is seen that photodesorption is a very efficient process for many semiconductors. The basic model developed over the years is presented and correlated with experimental results. Typical figures from important papers are reproduced. The reference list covers the international literature and is believed to be quite complete.

Robert J. Madix, Stanford University, California

#### Chemical Reactions on Single Crystal Metal Surfaces

The use of the techniques of flash desorption spectroscopy in conjunction with normal surface characterization methods to study the kinetics and mechanism of surface reactions is described. First, the methods by which activation energies and preexponential factors are obtained are discussed. Then, the extension of flash desorption to studies of surface reactions is presented. Examples, including oxidation reactions and catalytic reactions of simple hydrocarbons, are taken from the work of several investigators. Finally, the use of isotopic substitution for mechanistic analysis by thermal programmed reaction spectroscopy is described. The combined utility of these methods is exemplified by the decomposition of formic acid on a variety of metal surfaces and by the oxidation of ethanol on silver. These examples clearly illustrate the role of surface composition in altering the reactive behavior of metal surfaces.

John P. McTague, University of California-Los Angeles

#### Neutron Diffraction by Adsorbed Monolayers

The principles of neutron scattering, both elastic and inelastic, are discussed, particularly as they apply to the study of adsorbed thin films. Despite the fact that thermal neutrons are not surface specific (or even preferentially sensitive to surface layers), recent studies have shown that valuable and even unique structural and dynamic information can be obtained for coverages as low as a fraction of a monolayer. The most detailed work to date has been on simple films (He, H<sub>2</sub>, D<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, Ar, Kr) physisorbed on the [001] surface of graphite, but there has also been progress in determining the dynamics of hydrogen chemisorbed on metals. Representative examples

are discussed.

Dietrich Menzel, Technische Universität München, Germany

### Photoelectron Spectroscopy of Adsorption Layers

The use of photon-induced electron emission for the investigation of the properties of adsorption layers and the recent progress in this field are surveyed. The discussion is subdivided into core-level and valence-level photoemission. Core-level photoemission embraces the use of X-ray photoemission (XPS or ESCA and satellites) and X-ray-induced Auger electrons (XAES). The application for qualitative and quantitative analysis is described, as well as the differentiation of various surface species by utilization of the varying chemical shifts. The concept of chemical shift for surface species is discussed, as well as its inherent difficulties. The additional information which can be gained from satellite studies and from XAES is stressed. To date, valence-level photoemission has mostly been done using UV photoelectron spectroscopy (UPS), but can also be done with XPS and intermediate wavelengths (synchrotron radiation). The potentials and difficulties of this method for the characterization of valence levels of surface species and the information obtainable from wavelength and angle-dependent studies are discussed. The particular advantage to be gained from studies combining several of these spectroscopies is emphasized.

J. M. Morabito, Bell Laboratories, Allentown, Pennsylvania

### Compositional Depth Profiling by Auger Electron Spectroscopy

Depth profiling using Auger electron spectroscopy consists of measuring Auger peak heights as a function of time while sputtering. Compositional depth profiling is obtained by converting the peak heights into compositions using relative sensitivity factors and sputter times into depths using sputter rates. The biggest problems in converting peak heights to compositions are the matrix effects: escape depth ratio, backscatter correction factor, peak shape correction factor, and sputter correction factor. For cases where the peak shape factor can be ignored, the relative sensitivity factor is equal to the ratio of the peak heights in the pure metals multiplied by two terms. The first term involves the atomic densities, the escape depths, and the backscatter correction factors. These can all be obtained, and the combined term can be as large as a factor of four. This might cause, for example, a 10% concentration to be misinterpreted as a 2.5% concentration if the correction term is ignored. The matrix dependence of this term is rather small, however, typically less than 20%. Thus, if the proper correction is applied, the concentration might be  $10 \pm 2\%$ . The other term is the sputter correction factor, which as it can be as large as seven, should not be ignored either. In some cases, however, this term only varies by  $\pm 30\%$  with composition;



therefore, one correction factor is adequate over a large composition range. The sputter time is converted to depth using sputter rate data. If the composition is reasonably uniform, the time to sputter through a known thickness will suffice. Other methods are available for nonuniform composition, and these are also discussed. Accuracies are generally in the  $\pm 20\%$  range.

Neville G. Parsonage, Imperial College of Science and Technology,  
London, U.K.

#### Computer Simulation of Adsorption

Computer simulations of three-dimensional adsorption systems using Monte Carlo and molecular dynamics methods are reviewed. The Monte Carlo method, in both the Canonical and Grandt Canonical Ensembles, and the molecular dynamics method are briefly described with reference to their application to bulk systems. Special problems which occur on applying these techniques to adsorption systems are examined. In particular, problems which arise from the need to apply corrections for the long-range part of the intermolecular potential are explored. For the liquid-vapor interface, a brief account is given of the present views with regard to the existence of oscillations in the singlet distribution function. Three separate studies of the adsorption of noble gases on graphite, represented as a continuum, are described in detail. At coverages greater than one monolayer, it is shown that the Brunauer-Emmett-Teller theory for the adsorption isotherm is surprisingly good, although it is much poorer with respect to the build-up of the individual layers. The Polanyi potential theory is also fairly successful, in contrast to the "Slab" theory. At coverages below a monolayer, evidence for transitions is found, the nature and positions of these being, in general, in accord with experiments. Recent work employing a structured, rather than a continuum, surface for graphite is shown to lead to somewhat poorer agreement with the experimental adsorption isotherms. A discussion is given of the occurrence of metastability in the Monte Carlo simulations and the relationship of this to the molecular dynamics computations.

Lanny D. Schmidt, University of Minnesota

#### Surface Reactions at High Pressures

Industrial catalytic reactions are conducted at or above atmospheric pressure, and at these pressures, many phenomena can occur that are unimportant at lower pressures. Among the factors which must be considered in describing catalytic processes are (1) surface morphology changes caused by the reaction, (2) surface composition changes produced by relatively slow side reactions on the surface, (3) high local temperatures produced by reaction heat, and (4) diffusion and mass transfer resistances. Effects of these processes on surface reactions will be discussed and illustrated with laboratory examples. Recent



studies of surface morphologies of catalysts using scanning and transmission electron microscopy and of chemical composition using scanning Auger electron spectroscopy are summarized. Reaction kinetic measurements on polycrystalline and single crystal surfaces measured over wide temperature and pressure ranges are also considered. Implications of these processes with regard to the relation between atomistic characterization of surfaces and industrial catalytic processes is discussed.

F. C. Tompkins, Imperial College of Science and Technology, London, U.K.

#### Historical Review: Chemisorption on Metals - Retrospect and Prospect

This paper presents a historical review of the development of knowledge on the chemisorption of gases or metals since the concept of monolayer adsorption was put forward by Langmuir in 1916. Particular attention is directed towards the production, maintenance, and monitoring of surfaces that are free of contamination, thereby inaugurating the basis of all modern experimental work. The recognition of the importance of the geometric structure and its determination by LEED together with field and ion-emission microscopy are discussed before proceeding to the impact of electron spectroscopic techniques in obtaining information on the electronic properties of metal surfaces and chemisorbed overlayers. Some indication of the progress that may be expected in the near future in the understanding of chemisorption processes is then briefly outlined.

Tien T. Tsong, The Pennsylvania State University

#### Properties of Single Atoms on Metal Surfaces

A fundamental understanding of surface phenomena such as surface atom transport processes, nucleation and growth of crystals, surface reactivity, etc. requires a knowledge of the behavior of single atoms on solid surfaces. The diffusion parameters, the interatomic potential energy between two atoms, the binding energy with the substrate lattice, the surface induced dipole moment, the polarizability, and other basic properties of surface atoms can now be determined by investigations of a specified number of atoms on atomically well-defined crystal planes in the field-ion microscope. The principles and techniques for deriving these parameters are described and some of the existing results are summarized. The merits and limitations of the different techniques are compared and the interrelationship of the parameters are discussed.

Jan H. van der Merwe, University of Pretoria, Rep. of South Africa

The Role of Lattice Misfit in Epitaxy

Epitaxy is the phenomenon in which one crystal grows in a specific orientation(s) on another crystal even though their normal lattices may not fit at their interface. Lattice misfit, together with atomic bonding and crystal size, have a pronounced influence on epitaxy. The concept of misfit implies more than a difference in bulk lattice parameters. The misfit is usually accommodated jointly by misfit strain (MS) and misfit dislocations (MDs) or, in the limit of weak interfacial bonding, simply by a misfit vernier. The balance between the accommodation modes closely obeys an equilibrium minimum misfit energy  $E_m$  criterion, where  $E_m$  comprises contributions  $E_e$  and  $E_D$  from MS and MDs, respectively. The possibility that equilibrium conditions are not met and that interdiffusion may redistribute the misfit, MDs, and MS is briefly considered. The roles of  $E_e$  and  $E_D$  in the epitaxial orientating power of a substrate-overgrowth combination and in the epitaxial growth morphology are discussed with special reference to the relative strengths of overlayer-overlayer and overlayer-substrate bonds. Although much has already been achieved in the understanding of the various features of epitaxy, more exact models and more exact calculations are still needed.

Since the discussions are an essential part of ISISS, the Session Chairmen play an important role. At ISISS 1977, the following surface scientists served as Chairmen:

Dr. Vladimir Haensel  
Science & Technology  
UOP Inc.  
Des Plaines, Illinois

Professor Maurice B. Webb  
Department of Physics  
University of Wisconsin-Madison  
Madison, Wisconsin

Professor John Pritchard  
Department of Chemistry  
Queen Mary College  
London, England

Dr. Manfred S. Kaminsky  
Surface Science Center  
Argonne National Laboratory  
Argonne, Illinois

Professor W. Keith Hall  
Laboratory for Surface Studies  
University of Wisconsin-Milw.  
Milwaukee, Wisconsin

Dr. James S. Murday  
Office of Naval Research  
Washington, D.C.

Professor Richmond B. McQuistan  
Laboratory for Surface Studies  
University of Wisconsin-Milw.  
Milwaukee, Wisconsin

Professor Robert G. Greenler  
Laboratory for Surface Studies  
University of Wisconsin-Milw.  
Milwaukee, Wisconsin

Professor John D. Rogers  
Institute of Physics  
Universidade Estadual De Campinas  
Brasília



One hundred and fifty-six scientists from all parts of the U.S.A., from Brasil, Canada, Ecuador, Germany, Israel, Japan, the Rep. of South Africa, and the United Kingdom participated. They came from universities (76%), from industry (21%), as well as government institutions (3%). The educational value of the conference is demonstrated by the fact that 44% of the participants were Graduate Students and Post-Doctoral Fellows, the registration fee was kept as low as possible.

The following registration fees were requested:

Registration before July 22, 1977:

\$45.00 Regular

\$33.00 Graduate Students and Post-Doctoral Fellows

Registration after July 22, 1977:

\$55.00 Regular

\$45.00 Graduate Students and Post-Doctoral Fellows

Students in the UW-System payed a nominal fee.

Besides the scientific program, a number of social programs were arranged. They included a family program, dinner trous, a reception for speakers and participatns from foreign countries, and a banquet. Many participants used the opportunity to visit the facilities of the Laboratory for Surface Studies at UWM. In connection with the Summer Institute, an exhibition of surface science books was organized.

International scientific societies and journals announced the conference. About 2700 scientists were contacted directly.

As in the case of former ISISS, the papers presented are published in consecutive issues of CRC-Critical Reviews in Solid State and Materials Sciences under the title "Surface Science: Recent Progress and Perspectives (ISISS 1977). As in 1975, the journal publication will be followed by a CRC Monotopic book (one

volume, hard bound).

ISISS 1977 was supported by grants from the University of Wisconsin-Milwaukee and a combined grant from ONR-AFOSR.

As typical for the response of participants to ISSS 1977, statements will be quoted from two letters.

Professor F. C. Tompkins, FRS  
Imperial College of Science and Technology  
London, United Kingdom

"I shall greatly look forward to the printed version of the lectures which were of the high class and standard that has become the feature of these biennial meetings."

Professor J. P. McTague  
University of California-Los Angeles  
Los Angeles, California

"I am sure that by now many of the participants in ISSS 1977 have already thanked you for your efforts and those of your colleagues, which resulted in such an excellent Institute. It was one of the most informative and enjoyable conferences I have ever attended, and I just wish to add my own appreciation to the universally expressed sentiments I heard from others."

Dr. Ralf Vanselow  
Director, ISSS 1977